

# **A Molecular Dynamics Simulation Study of the Self-Diffusion Coefficient and Shear Viscosity of the Lennard-Jones Fluid**

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New simulation results for the self-diffusion coefficient and the shear viscosity of the Lennard-Jones model fluid will be presented. Extensive equilibrium molecular dynamics simulations were performed along sub- and supercritical isotherms from the low density gas up to the compressed liquid near the melting line. Both transport properties were obtained from their corresponding Einstein relations. Furthermore, the subdivision of the shear viscosity into the kinetic-kinetic, kinetic-potential and potential-potential contributions, which arises naturally in the time correlation function formalism, was investigated. The simulation procedure was validated by a series of simulations at fixed conditions close to the triple point which were investigated by other authors before. These simulations with different particle numbers and cutoff radii reveal a strong dependence of the kinetic-potential and potential-potential contributions on the cutoff-radius whereas the kinetic-kinetic contribution and the self-diffusion coefficient are rather insensitive against this parameter. The general simulations along isotherms were carried out with 1372 particles and cutoff radii  $r_c = 5.5$  or  $6.5$  over 1.5 to 2 million time steps. The presented viscosity data are substantially more accurate than earlier results. For the first time, the behavior of the three viscosity contributions was characterized over a broad range of fluid states and not only at selected state points. These results provide coherent insight into the nature of this transport property from a little-explored view angle.